

# Revisiting two holes in a locally antiferromagnetic background: the role of retardation and Coulomb repulsion effects

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The problem of two holes in the presence of strong antiferromagnetic fluctuations is revisited using computational techniques. Two-dimensional clusters and 2-leg ladders are studied with the Lanczos and Truncated Lanczos algorithms. Lattices with up to  $2 \times 16$  and  $\sqrt{32} \times \sqrt{32}$  sites are studied. The motivation of the paper is the recently discussed spatial distribution of holes in ladders where the maximum probability for the hole-hole distance is obtained at  $d = \sqrt{2}$  in units of the lattice spacing, a counter-intuitive result considering that the overall symmetry of the two-hole bound state is  $d_{x^2-y^2}$ . Here this effect is shown to appear in small ladder clusters that can be addressed exactly, and also in planes. The probability distribution of hole distances  $d$  was found to be broad with several distances contributing appreciably to the wave function. The existence of holes in the same sublattice is argued to be a consequence of non-negligible retardation effects in the  $t - J$  model. Effective models with instantaneous interactions nevertheless capture the essence of the hole pairing process in the presence of short-range antiferromagnetic fluctuations (specially regarding the symmetry properties of the condensate), similarly as the (non-retarded) BCS model contains the basic features of the more complicated electron-phonon problem in low temperature superconductors. The existence of strong spin singlets in the region where the two hole bound state is located is here confirmed, and a simple explanation for its origin in the case of planes is proposed using the Néel state as a background, complementing previous explanations based on a spin liquid undoped state. It is predicted that these strong singlets should appear regardless of the long distance properties of the spin system under consideration, as long as the bound state is  $d_{x^2-y^2}$ . In particular, it is shown that they are present in an Ising spin background. The time retardation in the family of  $t - J$  models leads naturally to low-energy hole states with nonzero momentum and spin one, providing a possible explanation for apparent  $SO(5)$ -symmetric features observed recently in this context. Finally, the influence of a short-range Coulombic repulsion is analyzed. Rough estimations suggest that at a distance of one lattice spacing this repulsion is larger than the exchange  $J$ . The hole distribution in the  $d_{x^2-y^2}$  bound state is reanalyzed in the presence of such repulsion. Very short hole-hole distances lose their relevance in the presence of a realistic hole-hole interaction.

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## I. INTRODUCTION

Among the most appealing scenarios to explain the behavior of the high temperature superconducting compounds are those based on antiferromagnetic fluctuations as the mechanism for hole pairing. These ideas have been formulated over the years in a variety of contexts. Early diagrammatic work for heavy fermions in the presence of antiferromagnetic correlations suggested that magnon interchange can lead to  $d$ -wave pairing [1]. The nearly antiferromagnetic Fermi liquid proposal arrives to the same conclusion also in a diagrammatic context where low-energy spin excitations are assumed to coexists with holes [2]. Since in real doped cuprates the antiferromagnetic correlation length  $\xi_{AF}$  is only of a few lattice spacings other approaches have emphasized the relevance of the short distance physics in the problem [3]. Independently of these approaches which are based on the resum-

mation of particular sets of Feynman diagrams, a vast amount of computational work has been devoted to the interaction of holes with spin excitations [4]. Although these techniques have as a natural limitation the finite size of the clusters that can be studied, they have the important advantage that inside these clusters the information gathered is basically exact. Since  $\xi_{AF}$  is small in the cuprates, and, in addition, experimental estimations of the coherence length also suggest small size Cooper pairs [5], computational approaches are very important to clarify the physics of carriers in a fluctuating antiferromagnetic background. Following these ideas the existence of pairing of two holes in the  $d_{x^2-y^2}$  channel using the  $t - J$  and Hubbard models was observed since the early theoretical studies of the cuprates [4,6]. For realistic values of  $J/t$  the size of the pair has been known to be small, of only a couple of lattice spacings at most [7]. In addition, recent work in the limit where the attraction

between holes is assumed much larger than the bandwidth provided a real-space simple qualitative picture for the formation of  $d_{x^2-y^2}$  bound states [8]. It turns out that not only a suitable effective potential between holes is needed to obtain pairs in the  $d$ -channel (repulsive on site, and attractive between nearest-neighbors) but in addition the form of the dispersion of holes renormalized by spin fluctuations plays an essential role in stabilizing  $d$ -wave pairing instead of extended  $s$ -wave pairing [8].

The small tight pairs found numerically suggest that the cuprates are in an intermediate regime between the BCS limit, where the pair size is much larger than the mean distance between carriers, and the Bose condensation regime defined in the opposite limit. Recent experimental work reporting the presence of pseudogap features in the normal state of the underdoped cuprates [9] have revived the possibility that hole pairs may exist above the superconducting critical temperature, at least as finite lifetime fluctuations [10]. These results provide extra support to the idea that a “real-space” approach to hole pair formation is more enlightening than a momentum-space approach. In the context of holes in antiferromagnets it is natural to propose an effective model for holes where these particles move within the same sublattice (as suggested by a variety of studies of the one hole problem in an antiferromagnet), interacting through an effective potential induced by antiferromagnetism [11]. In the limit where this potential is assumed to be short-ranged the presence of  $d$ -wave bound states has been deduced analytically through the solution of the two-body problem, and the presence of superconducting correlations has been found using the BCS mean-field approach with RPA fluctuations supplemented by numerical studies [8]. More recent work has extended these ideas to include the interchange of magnons, leading to a longer range effective potential between holes reaching similar conclusions regarding the  $d$ -wave pair formation in the problem [12].

Recently, a complementary approach to the study of holes in the cuprates has been considered. It is based on the analysis of even-leg ladder systems [13] since they have a robust spin gap, a feature that is also present in the normal state of underdoped cuprates. The 2-leg ladder has an antiferromagnetic correlation length of about 3 lattice spacings [14], similar to the correlation observed in the doped cuprates. Then, ladders have coexisting spin gap features and short-range antiferromagnetism. In this context it has been observed that a couple of holes introduced in the 2-leg ladder form a bound state for realistic values of  $J/t$  with characteristics of a  $d$ -wave pair [15,16] (although strictly speaking a sharp distinction between  $d$ - and  $s$ -wave pairs does not exist in ladders). While the main reason for the hole attraction is the minimization of broken rung singlets [17], the appearance of a  $d$ -wave character in the pairing is likely caused by the presence of short-range antiferromagnetic fluctuations, establishing an interesting analogy between planes and ladders.

Recent work in this context using the Density Matrix Renormalization Group (DMRG) [18] approach has con-

firmed the presence of two hole bound states in the  $d$ -channel in the case of 2-leg ladders [19]. However, in this study it was remarked that holes in the bound state spend part of the time located along the diagonals of the elementary plaquettes in the problem, a feature somewhat counter-intuitive for  $d$ -wave pairs since a two-body problem with  $d_{x^2-y^2}$  character cannot have particles in such a configuration. In addition, the presence of strong spin singlets in the vicinity of holes, resembling the Resonating Valence Bond (RVB) states characteristics of spin liquids [20], were noticed. In ladders an explanation for these results was proposed in Ref. [19]: the singlets along plaquette diagonals have frustrating character and pairing occurs to share frustration. As a consequence of this effect domain walls are induced in the problem. A similar numerical result in the context of two-dimensional planes was earlier reported using Exact Diagonalization (ED) techniques on small clusters [21].

The above mentioned recent numerical studies motivated in part the present paper. Its purpose is to further analyze the two hole problem in planes and 2-leg ladders using Exact Diagonalization [4] and Truncated Lanczos [22] algorithms, as well as to propose intuitive arguments to explain the results observed in the present and previous investigations. The physics obtained with the DMRG method on ladders [19] is found to be contained also in small clusters that can be handled exactly. An intuitive picture both in real and momentum space is provided to justify how holes can exist in the same sublattice in a  $d_{x^2-y^2}$ -wave bound state. The importance of *retardation* effects for this feature is remarked, and thus it is unavoidable to conclude that time-dependent hole-hole potentials are needed to quantitatively account for the physics of the  $t - J$  model. However, effective models with instantaneous interactions are expected to capture most of the relevant physics, specially regarding the symmetry of the condensate, similarly as the BCS model does for the electron-phonon problem. The existence of strong spin singlets in the immediate vicinity of tightly bounded holes on planes is here argued to be caused, at least in part, by the  $d$ -character of the bound state and its existence is independent of the special features of the spin background. In particular they exist in the case of an Ising background, which does not have quantum fluctuations. For the case of ladders, since spin singlets are already formed in the undoped system our proposed explanation only addresses the unexpected strong strength of some particular spin singlets, and it is thus complementary to previous explanations [19]. It is also reported here that the special configuration where holes are located at short distances, such as  $\sqrt{2}$  lattice spacings, is just one of several equally important hole distances in the two hole problem, and in addition it becomes unstable after the introduction of a realistic nearest-neighbor (NN) Coulombic repulsion.

## II. HOLES IN SAME SUBLATTICE IN BOUND STATES TRANSFORMING AS $X^2 - Y^2$

### A. Discussion in Real Space

As explained in the Introduction, previous studies [21,19] have emphasized that the configuration where the two holes are located in the same sublattice across the diagonals of a plaquette has a substantial weight in the two-hole ground state. At first sight this result seems counter-intuitive since one is used to the naive notion that in the  $d_{x^2-y^2}$  subspace the wave function of two particles has a node along the lattice diagonals. However, remember that this picture is based on the idealization of the two-hole problem in a spin background (which is a  $N-2$  body problem, where  $N$  is the number of sites of the cluster under consideration) as a system of only two particles in an otherwise empty lattice interacting through a static effective potential. This potential is staggered in real space (peaked at  $(\pi, \pi)$  in momentum space), favoring the location of holes in opposite sublattices. A wide variety of calculations including diagrammatic techniques supplemented by Quantum Monte Carlo studies [6],  $t-J$  model estimations [4], and other approaches [12] all agree in this respect. Using such a hole-hole potential there is no doubt that the two particles *must* be located in opposite sublattices for the  $d_{x^2-y^2}$  symmetry to be realized. Even within the context of the full  $t-J$  model, if it were possible to “integrate out” the spin degrees of freedom, the resulting potential between the two holes at zero frequency must again induce the same feature.

For the case of planes, the key ingredient to understand the apparent discrepancy between the numerical and analytical calculations detailed above are the *retardation* effects caused by the finite velocity propagation of the spin excitations in lightly doped antiferromagnets. As a simple example consider a couple of holes located next to each other in a perfect Néel spin background, as shown in Figs.1a-b. To construct a  $d_{x^2-y^2}$  wave function in this context, it is necessary to combine Fig.1a and 1b with a negative relative sign. This provides the simplest example in the two hole subspace of a contribution to the  $d_{x^2-y^2}$  bound state. If the Néel state is considered as the reference “vacuum”, then each hole at site  $i$  can be formally assigned an effective spin according to the definition  $S_i^{eff} = S_i - S_i^{AF}$ , where  $S_i$  is zero for a hole and  $S_i^{AF}$  is the spin of the reference state at the same site. With this definition holes at distance of one lattice spacing have opposite effective spins. However, there are other contributions to the many-body ground state of two-holes in the  $d_{x^2-y^2}$  subspace caused by the presence of a nontrivial spin background. For example, Fig.1c illustrates what occurs if a hole is moved by one lattice spacing from its position in Fig.1a. In this situation the spin that is moved in the opposite direction of the moving hole is now located in the wrong sublattice with respect to the background. Once again if the Néel state is de-

fined as the reference vacuum, such an arrangement of holes and spins is represented as in Fig.1d showing that it corresponds now to a *three-body* problem. The holes being now in the same sublattice have the same spin projection according to the definition of the spin  $S_i^{eff}$  given above, and the overall spin conservation is achieved by realizing that the actual spin involved in the hole hopping process, which now lives in the wrong sublattice, plays the role of a spin *one* excitation with respect to the Néel background. Thus, the hole hopping in the lightly doped  $t-J$  model can be rephrased as the destruction of a hole with spin  $\sigma$ , and the creation of a hole with spin  $-\sigma$  and a bosonic excitation of spin  $2\sigma$  (Note that the pair operators introduced in Ref. [21] also contains the notion that spin excitations are needed to have  $d$ -wave symmetry in this context). Formally this corresponds to a hopping process regulated by the Hamiltonian

$$H_{hopp} \propto \sum_{i, \mu=\pm\hat{x}, \pm\hat{y}, \sigma} (c_{i+\mu, -\sigma}^\dagger c_{i, \sigma} a_{i, 2\sigma}^\dagger + h.c.) \quad (1)$$

where the  $c$ -operators represent the (fermionic) holes, and the  $a$ -operators the (bosonic) spin one excitations. The rest of the notation is standard. Once the three-body character of the problem is understood, it is easy to find combinations of individual states that transform globally as  $x^2 - y^2$ . For instance, Fig.1e contains four states with holes located along the diagonal of a plaquette coexisting with a spin excitation as described before. If the four states have equal absolute weight but the relative signs indicated in Fig.1e, then it can be shown that a  $d_{x^2-y^2}$  state is formed. This reasoning has been tested by solving a  $3 \times 3$  cluster exactly fixing one hole at the center and allowing for a second one to orbit around. Simply considering the dominant configurations in the ground state, the three-body characteristics of the motion of two holes around each other become clear. In addition, certainly the discussion based on Figs.1a-e can be extended to distances larger than those involved in a single plaquette. Actually as  $J/t$  is reduced in the two hole problem, longer and longer distances between the holes will have larger weights in the wave function since  $J/t$  regulates the strength of the attraction.

Based on this reasoning the computational results [21] reporting that in planes the configuration with holes located in the same sublattice has the largest weight in the two hole ground state can be rephrased as an indication that the spin excitations are not “instantaneous” from the point of view of the holes, but instead they have a finite lifetime. In other words, the process of holes moving within a given sublattice is not a rapid tunneling process. “Retardation” effects apparently are important in models where antiferromagnetic correlations at short distances are robust. This is not too surprising considering that a typical spin wave velocity is regulated by the exchange  $J$  while a variety of numerical results have shown that the quasiparticle bandwidths in the  $t-J$  and related models for cuprates are also of order  $J$ , at least in the

underdoped regime [4].

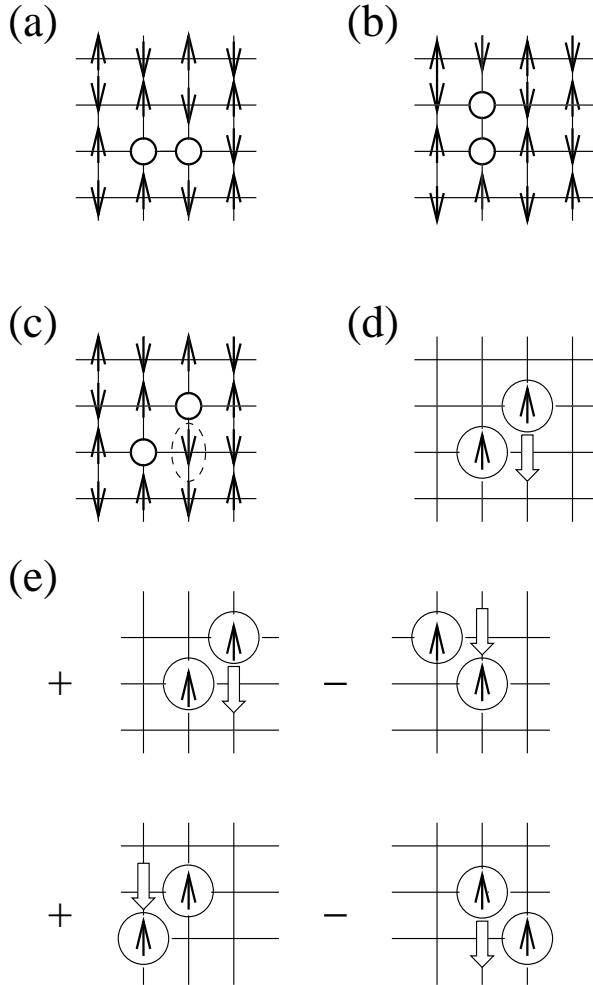


FIG. 1. (a-b) Pictorial representation of a couple of holes in a spin Néel state; (c) The movement of a hole in (a) introduces a spin incorrectly aligned with respect to the staggered order in the background; (d) Taking the Néel state as reference (c) corresponds to a three body problem, namely two holes and a spin excitation; (e) The three bodies of (d) can be arranged in a  $d_{x^2-y^2}$  state as indicated.

Note that the effect presented here is “local” in the sense that it involves just a few sites of the lattice. Thus, naming the spin excitation of Fig.1c as a spin-wave, which is usually associated to a delocalized object, is somewhat misleading since a localized excitation can actually be decomposed into plane waves carrying a similar weight for all momenta. Since the density of states of magnons peaks at  $\mathbf{k} = (\pi/2, \pi/2)$ , these states may matter more for local processes than the low-energy extended excitations of momentum  $(\pi, \pi)$ . This is similar to what occurs in electron-phonon problems where the phonons at the Debye frequency are more relevant than the low-energy acoustic modes. Then, the spin-wave velocity (which is defined in the vicinity of  $(\pi, \pi)$  for spin problems) is likely not the most important quantity to

judge effects of retardation in the formation of tight hole pairs.

## B. Strong spin singlets along plaquette diagonals: an intuitive explanation

The DMRG studies of Ref. [19] for the case of two holes located at distance  $\sqrt{2}$  also reported the existence of a strong spin-singlet along the diagonal the opposite to the one where the holes are located (for other recent studies see Ref. [23]). In the context of ladders their existence was argued to be caused by the presence of frustrating singlet effects [19]. In addition, singlets are already formed in the ground state of 2-leg ladders and, thus, it is natural that they contribute to the movement of holes. However, the strong strength of these “diagonal” singlets is unusual, and even more strange is that they also appear in two-dimensional clusters as shown numerically below. Then, the authors believe that there must be some other ingredient contributing to the existence of these strong diagonal singlets. The discussion of the previous subsection allow us to propose an explanation based on holes in an antiferromagnetic background that complements previous discussions [19] based on spin liquid states. Consider once again Figs.1a-b remembering that these two states enter in the wave function of a  $d_{x^2-y^2}$  state with opposite signs. Moving the right hole in Fig.1a up one lattice spacing, Fig.1c is obtained where the spins along the diagonal opposite to the holes have opposite  $z$ -projections. This is once again reproduced in Fig.2a. Now consider Fig.1b and move the upper hole to the right one lattice spacing: in this case (Fig.2b) the spins along the diagonal opposite to the holes are again antiparallel, but with projections spin inverted with respect to those found in Fig.2a. Next, combine Fig.2a and 2b taking into account the fact that Figs.1a-b have a weight of opposite sign in the ground state, and that the spins not belonging to the plaquette being analyzed have not changed. Then, it is clear that a *spin singlet* along the diagonal opposite to the holes is formed, as illustrated in Fig.2c. Note that this reasoning should work specially well in an Ising background (i.e. using a Néel state without quantum fluctuations), and in Sec.III numerical results confirm this prediction using the  $t - J_z$  model [24]. Note also that for the case of an extended  $s$ -wave, the same line of arguments would lead to a *triplet* along the diagonal, a prediction that will be tested numerically below.

A similar reasoning helps in understanding why singlets are formed next to hole pairs even if they are not along diagonals. Consider Fig.1b and move the upper hole first to the right and then down one lattice spacing. The resulting spin configuration is shown in Fig.2d. Combining this state with Fig.1a and, again, remembering that Figs.1a and 1b had a weight of opposite sign, now Fig.2e is obtained. Then, the presence of singlets next to

holes is also natural when  $d_{x^2-y^2}$  states are considered, and they are there regardless of the overall ground state properties of the spin system.

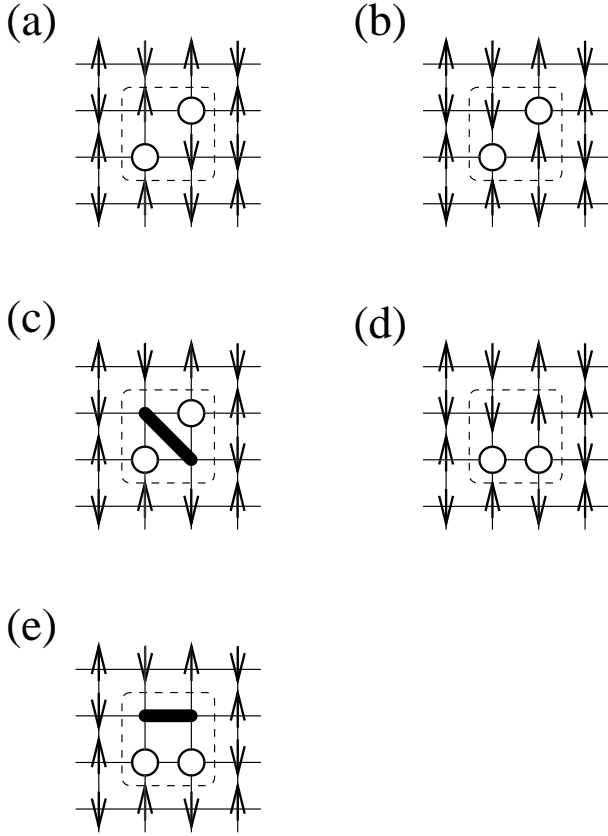


FIG. 2. Spin and hole configurations allowing us to show that strong spin singlets are expected in the vicinity of holes orbiting in a  $d_{x^2-y^2}$  state when a Néel background is considered. For details see the text.

### C. Discussion in momentum space

The previous discussion carried out in real-space in the limit where holes are heavy can be reinterpreted using a diagrammatic approach in momentum-space considering fermions (holes) interacting through the exchange of bosons (spin excitations). Fig.3a contains a “randomly” selected diagram contributing to the bound state of two holes in a spin background. The important point to remark arises if a snapshot of the system at an arbitrary time (such as the one indicated by the dashed line) is taken: in this case it is clear that together with the pair of fermions there may be a nonzero number of spin excitations. In spite of this increase in the number of particles at intermediate times, all must be combined in such a way that the original spin and symmetry under spatial rotations of the fermionic pair at time  $t = -\infty$  is conserved. In the case of relevance for the two-hole bound state the total momentum and spin must remain zero, and the  $d_{x^2-y^2}$  symmetry under rotations must be pre-

served. Consider the intermediate time denoted by the dashed line in Fig.3a: in this situation one vertex interaction has taken place at previous times, changing the spin of the fermion involved, and now both fermions have the same spin projection with the boson carrying the compensating spin, as in the real-space picture of Fig.1d. In addition, if the boson has momentum  $\mathbf{q}$ , the holes originally in  $-\mathbf{k}$  and  $\mathbf{k}$ , now switch to  $-\mathbf{k}$  and  $\mathbf{k} - \mathbf{q}$ . At this intermediate time and if *only* the holes are considered one may arrive to the counter-intuitive conclusion that they have switched to a state of spin 1 and momentum  $q$ , that in addition is not in the  $d_{x^2-y^2}$  subspace (in principle they can be in any irreducible representations of the  $C_{4v}$  symmetry group of the square lattice). Such a conclusion would be incorrect since the overall quantum numbers are given by the combination of fermions and bosons. Concentrating on the behavior of only the fermions in the problem may lead to apparent paradoxes, as described before.

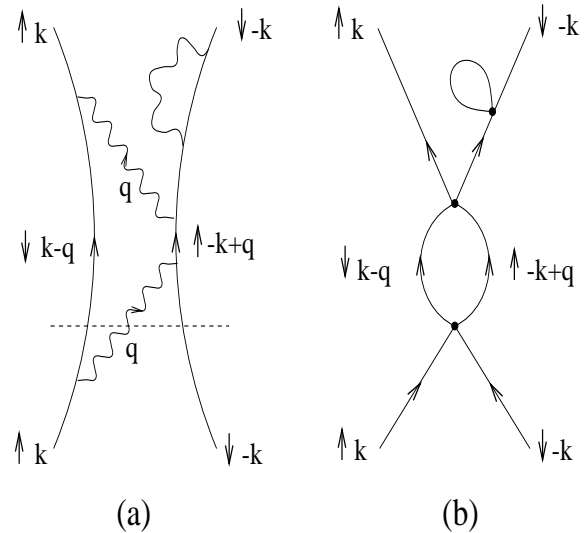


FIG. 3. (a) Momentum space representation of the interaction of two holes (solid lines) mediated by spin-waves (wavy lines). Spin and momenta are indicated. The dashed line represents an intermediate time relevant for the discussion in the text. Time runs upwards in the graph; (b) The same Feynman diagram as in (a) but now assuming that the interchange of spin-waves is instantaneous (no retardation). This collapses the spin-wave propagators into a point. Momenta and spin are indicated.

If the bosonic mediated interaction is considered instantaneous, i.e. when a  $\omega = 0$  potential is used to describe the hole-hole interaction, then a situation where at all times the holes carry the quantum numbers they had at  $t = -\infty$  is recovered (see Fig.3b). In this case, holes must necessarily reside on opposite sublattices for its bound state to transform as  $x^2-y^2$ . Then, it is the fact that the  $\omega \neq 0$  effects (retardation) cannot be neglected in the  $t - J$  model that allows for hole configurations belonging to the same sublattice. The diagrams in Figs.3a

and 3b are similar to those arising in the context of low temperature superconductors where electron-phonon interactions lead to pairing. Fig.3a is the analog of an interaction mediated by a phonon propagating slowly relative to the fermions, at a velocity regulated by the Debye frequency, while Fig.3b plays the role of a diagram using only the BCS model where the effective interaction is assumed to be instantaneous and attractive. Note that in principle this is a drastic approximation since the ratio of typical fermionic to phononic velocities is about 100 in the low temperature superconductors. Nevertheless, in this context it is known that the BCS model captures the essence of the electron-phonon interaction, in particular the  $s$ -wave symmetry of the superconducting condensate. Thus, it is reasonable to believe that a similar situation will occur in models for the Cu-oxides based on the interaction between holes and spin-waves where the relevant ratio of velocities is likely of order 1 (since both are dominated by  $J$  in the low hole density limit, as explained before). In other words, assuming that the interaction mediated by the spin-excitations is instantaneous is an approximation that preserves the relevant qualitative features of the problem, as the BCS model does in the electron-phonon problem. In this respect is that models of high- $T_c$  such as those proposed in Ref. [11], where it is claimed that a peak in the density of states of strong correlation origin causes the appearance of an “optimal” doping, can be qualitatively correct and useful as a starting point to understand spin-wave mediated superconductivity. However, for a quantitative analysis the full spin-hole problem with retardation effects included must be taken into account, and that should be the main message extracted from the numerical studies discussed here.

#### D. Implications for SO(5) scenarios

Note that the results of this section have implications for the recently proposed SO(5) scenario for the cuprates [25]. Once again if a snapshot of the system is taken at the intermediate time (dashed line) of Fig.3a the holes will be found to be in a triplet state of momentum  $\mathbf{q}$ , and this state will have low-energy. However, as discussed before even though the lower energy spin-waves appear at  $\mathbf{q} = \mathbf{Q}$ , their number is maximized at  $\mathbf{q} \sim (\pi/2, \pi/2)$  and, thus, no particular value of the momentum is *a priori* more important than others. This conclusion is in disagreement with the results of Ref. [25] that favor  $\mathbf{q} = \mathbf{Q}$  over other momenta. In Fig.4, the energies of the two-hole ground state as a function of momenta for the cases of a total spin zero and one and using the  $t - J$  model are given. The results are exactly calculated using a 18 site square cluster. In the triplet branch there is no major difference between the different momenta, in agreement with our discussion. The particular value  $\mathbf{q} = \mathbf{Q}$  is not specially important in a broad range

of couplings from  $J/t = 0.2$  to 1.6. The present reasoning is simple and avoids the use of complicated approximate symmetries of the  $t - J$  and Hubbard models [26].

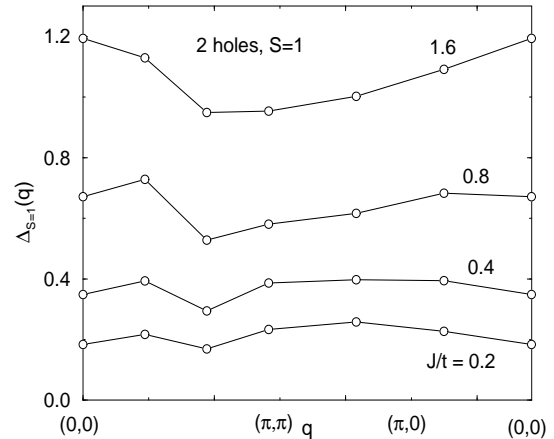


FIG. 4. Energy  $\Delta_{S=1}(\mathbf{q})$  of the state with the lowest energy in the subspace of two holes, momentum  $\mathbf{q}$ , spin one, and parametric with  $J/t$ . The energies are referred to the overall ground state energy of two holes, which is a zero momentum spin singlet. The results are obtained exactly using an 18 site cluster. Results for 20 sites are very similar.

### III. EXACT DIAGONALIZATION

#### A. Ladders

Here it is addressed numerically whether the recent DMRG results [19] for the behavior of two-holes in the ladder  $t - J$  model can be reproduced with other techniques. In particular, it would be desirable to obtain similar results in clusters accessible to Exact Diagonalization (ED) methods since the implementation of this algorithm is simple, calculations on a variety of  $t - J$ -like models can be carried out without much effort, periodic boundary conditions can be implemented, and dynamical properties can be analyzed.

Using the ED method let us first investigate the relative distance between holes in the case where two-hole bound states are expected. Fig.5 shows exact results obtained on a  $2 \times 10$  cluster with 2 holes and periodic boundary conditions. The probability  $P(d)$  of finding the holes at a relative distance  $d$  is presented against the coupling  $J/t$ . At every coupling, results are normalized such that  $\sum_d P(d) = 1$ . It is clear from the figure that for realistic values of  $J/t$ , such as 0.3 or 0.4, the highest chances indeed occur when  $d = \sqrt{2}$  is the hole separation. Thus, DMRG and Lanczos techniques provide similar results regarding this issue which is gratifying. However, Fig.5 provides extra interesting information:  $P(\sqrt{2})$  is actually similar to  $P(1)$  and, thus, results in this context must be necessarily interpreted in a probabilistic sense

i.e. the distance with the highest chances is not necessarily much relevant for the problem. For instance, note that  $P(\sqrt{2}) \approx 0.28$  which is substantially smaller than 1.

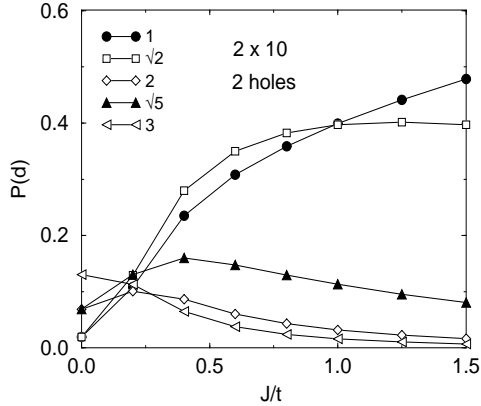


FIG. 5. Exact Diagonalization results using a  $2 \times 10$  cluster with two holes.  $P(d)$  is the probability of finding the holes at a distance  $d$  apart (convention indicated in the figure). Results for several couplings  $J/t$  are shown.

This is better illustrated in Fig.6 where  $P(d)$  at a fixed  $J/t$  is provided once one of the holes is fixed to an arbitrarily selected site of the 2-leg ladder. Working at  $J/t = 0.8$  the second hole is mostly located on the chain the opposite to the first hole, more specifically in the three sites the closest to it. As  $J/t$  is reduced to 0.4, the second hole spreads further its wave function and the largest probability is at distance  $\sqrt{2}$ . However, visually it is clear that a better representation is to imagine the hole as moving freely within a small region in the vicinity of the fixed hole, rather than assign special importance to one of the possible distances in this region. In addition, note that in the results of Fig.5, and considering data for other couplings not shown explicitly, no abrupt changes were observed as a function of  $J/t$  for the hole distribution and smoothly the size of the hole pair wave function grows as  $J/t$  is reduced. Finally at  $J/t = 0.2$  the second hole seems delocalized on the whole ladder (suggesting the absence of binding, or a bound state of size larger than the cluster considered here).

The DMRG studies [19] isolating the configuration of holes where they are located along the diagonal of a plaquette have also shown the existence of a strong spin singlet across the opposite diagonal of the same plaquette. A possible contribution to this result based on the  $d$ -character of the two-hole state was provided in Sec.II. As in the previous paragraphs, first it would be interesting to investigate if similar numerical information is obtained using ED techniques. In Fig.7 results are presented once again on a  $2 \times 10$  cluster and with two holes. The bonds where the spin correlation  $\langle \mathbf{S}_i \cdot \mathbf{S}_j \rangle$  has changed substantially compared with the undoped case are highlighted, following a convention similar as used in Ref. [19]. At large  $J/t$ , and isolating the configuration

where the two holes are in the same rung (since it has the highest chances) the spins along the nearest-neighbor rungs form a stronger spin singlet than in the undoped ladder. At  $J/t = 0.4$ , and now with two holes in the  $\sqrt{2}$ -configuration, the ED results confirm the previous DMRG calculations since indeed a robust spin singlet is found in the same plaquette where the holes are located. The considerable strength of the diagonal spin singlet naturally weakens the bonds that link the plaquette being analyzed with the rest of the ladder. If  $J/t$  is further reduced to 0.2, now the most likely hole configuration have the holes at distance  $\sqrt{5}$ . Concentrating on such configuration, it is interesting to notice that here there are two spin singlets along the plaquette diagonals (see Fig.7). Both are strong, causing the bonds between them to be weaker than in the undoped case. However, appealing as this picture may seem, the results in Fig.6 suggested that the holes are basically unbounded for this coupling. Thus, extracting conclusions out of snapshots of hole configurations is somewhat risky.

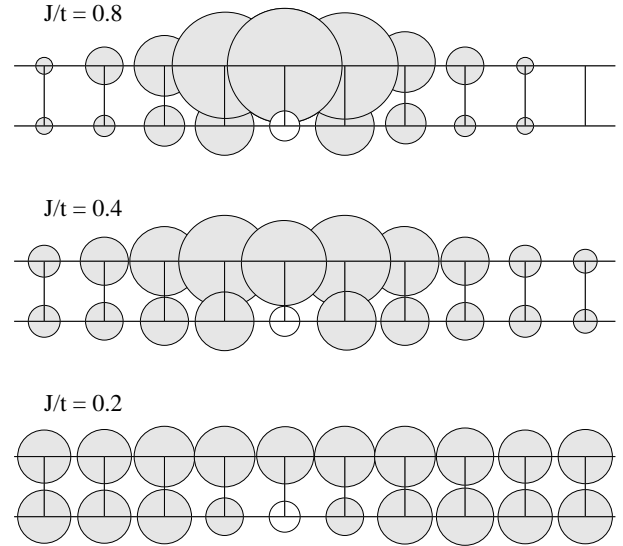


FIG. 6. Ground state results obtained on a  $2 \times 10$  cluster with two holes solved exactly. One hole is fixed at the position denoted by the open circle. The area of the gray circles is proportional to the probability of finding the other hole at a particular site. Results for several couplings are shown.

As a partial summary, in this section it was found that (i) ED techniques reproduce the pattern of spin singlets found previously in DMRG studies once the position of holes are fixed, but (ii) several other hole configurations have comparable probabilities. The two hole bound state for realistic values of  $J/t$  has a finite size and it resembles a bi-spin-polaron, with two particles moving quasi-freely inside a region of space regulated by the coupling. There are no sharp hole distances dominating the ground state of the problem. The spins inside the two-hole wave function form strong spin singlets which is natural since in

the undoped case the ground state has an RVB character. However, it was here argued that the  $d$ -wave properties of the state contribute at least in part to the strong spin singlet formation.

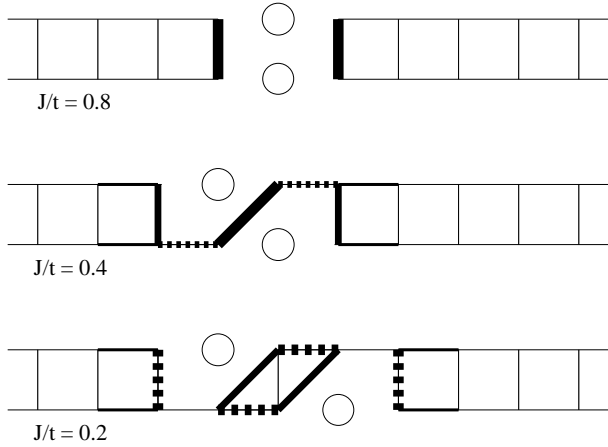


FIG. 7. Results for two holes obtained at several couplings  $J/t$  on a  $2 \times 10$  cluster solved exactly. The holes are fixed at the position with the highest chances in the ground state. Working in this subspace, bonds where the nearest-neighbor spin-spin correlation has the largest variation with respect to the undoped case are indicated. Solid (dashed) bonds indicate correlations which are larger (smaller) than in the undoped case by an amount larger than 20%. The thickness of the lines is proportional to the change observed.

## B. 2D clusters

Calculations similar as those in the previous subsection are here repeated using finite two-dimensional clusters. Fig.8 shows  $P(d)$  for a  $\sqrt{20} \times \sqrt{20}$  cluster solved exactly.

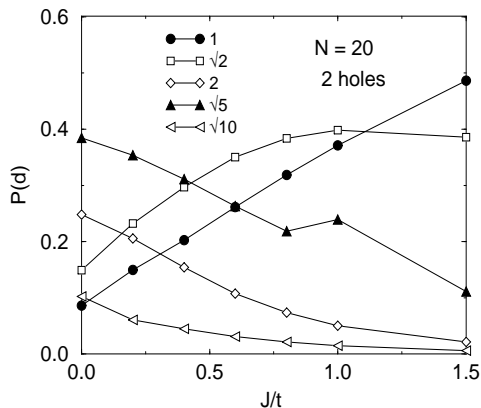


FIG. 8. Exact Diagonalization results using a 20 sites square cluster with two holes.  $P(d)$  is the probability of finding the holes at a distance  $d$  apart (convention indicated in the figure). Results for several couplings  $J/t$  are shown.

As in the case of the 2-leg ladders, a finite window in  $J/t$  exists where the distance  $d = \sqrt{2}$  has the highest chances, in agreement with Ref. [21]. However, if  $J/t = 0.3$  or  $0.4$  is considered realistic, then holes at  $d = \sqrt{5}$  have the largest probability. However, as in the case of ladders there are several distances with similar weight i.e.  $P(d)$  is not sharply peaked at one particular value of  $d$ . Actually, Fig.9 provides a pictorial representation of the probability of having one hole at a given position once the other hole is fixed at an arbitrary site, at three values of  $J/t$ . As in the case of ladders, for large  $J/t$  the wave function of the second hole is localized in the immediate vicinity of the first one. Reducing  $J/t$  the extension of the wave function smoothly increases, and at  $J/t = 0.2$  it covers the whole cluster suggesting the absence of a bound state. Thus, it seems that the bound state of two holes in 2-leg ladders and planes share many similarities, at least in the regime of small and intermediate size pairs. This universality may be caused by the presence of robust antiferromagnetic correlations in both systems. The bound state main features seem independent of the long distance (gapped vs gapless) characteristics of the undoped ground state.

The study of the pattern of spin singlets near holes shown in Sec.III.A can be repeated for the 2D clusters as well, and results are given in Fig.10. At large  $J/t = 1.6$ , the holes are located with the highest chances at a distance of one lattice spacing. As in the case of 2-leg ladders, the bonds parallel to the location of the holes contain strong spin singlets, which weakens the neighboring bonds along the same direction. When  $J/t$  is reduced eventually having the holes along a plaquette diagonal becomes the configuration with the highest chances (with the caveats of the previous paragraphs). In this case the spin singlet along the diagonal the opposite to where the holes are located is very strong, and as a consequence the other bonds associated with this spin singlet are weak, as it occurs for ladders. At small  $J/t = 0.2$ , once again two strong spin singlets are found between the holes which themselves have the highest chances of being located at distance  $\sqrt{5}$ , again similarly as observed for the same coupling on ladders.

A possible explanation for the presence of strong singlets was provided in Sec.II where it was proposed that they arise as a natural consequence of the  $d_{x^2-y^2}$  symmetry of the two-hole ground state in a Néel background. To verify this statement, ED studies for the spin anisotropic  $t - J$  model were carried out. In this case the Heisenberg  $\mathbf{S}_i \cdot \mathbf{S}_j$  interaction is replaced by  $S_i^z S_j^z + \lambda(S_i^x S_j^x + S_i^y S_j^y)$ . If  $\lambda = 1$  ( $\lambda = 0$ ) the Heisenberg (Ising) limit is recovered. Working at  $J/t = 0.6$  as an example, on 16 and 20 site clusters, and concentrating on two holes in the  $d_{x^2-y^2}$  subspace [27] at distance  $\sqrt{2}$ , the numerical results show that as  $\lambda$  is reduced from 1 to 0 the  $\langle S_i^z S_j^z \rangle$  correlation (along the diagonal the opposite to where the holes are) is negative, of similar value in this interval of  $\lambda$  (e.g. on the 20 site cluster,  $\langle S_i^z S_j^z \rangle \sim -0.21$  at  $\lambda = 0$  and  $\sim -0.19$



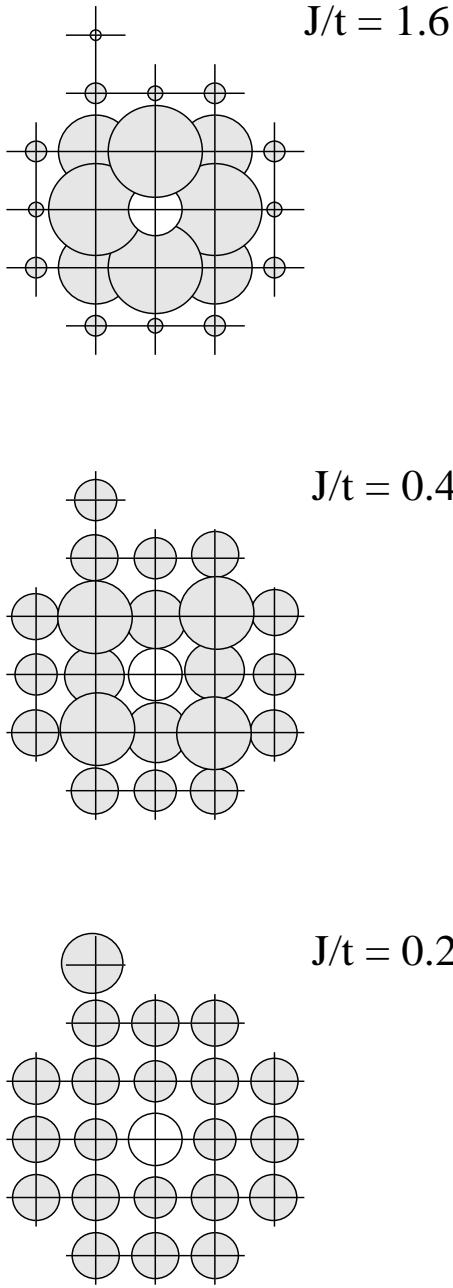


FIG. 9. Ground state results obtained on a 20 sites square cluster with two holes at  $J/t = 1.6, 0.4$ , and  $0.2$  solved exactly. One hole is fixed at the position denoted by the open circle. The area of the gray circles is proportional to the probability of finding the other hole at a particular site. More than 20 sites in the clusters are shown for clarity (periodic boundary conditions were used).

at  $\lambda = 1$ ). The value of the correlation changes smoothly as a function of  $\lambda$  implying that at least in part the presence of strong diagonal singlets in the Heisenberg limit is indeed caused by effects contained in Néel backgrounds, as explained in Sec.II. Very similar results have also been obtained for the  $t - J_z$  model on a  $2 \times 8$  ladder: consid-

ering  $J/t = 0.4$  as example,  $\langle S_i^z S_j^z \rangle \sim -0.21$  at  $\lambda = 1.0$

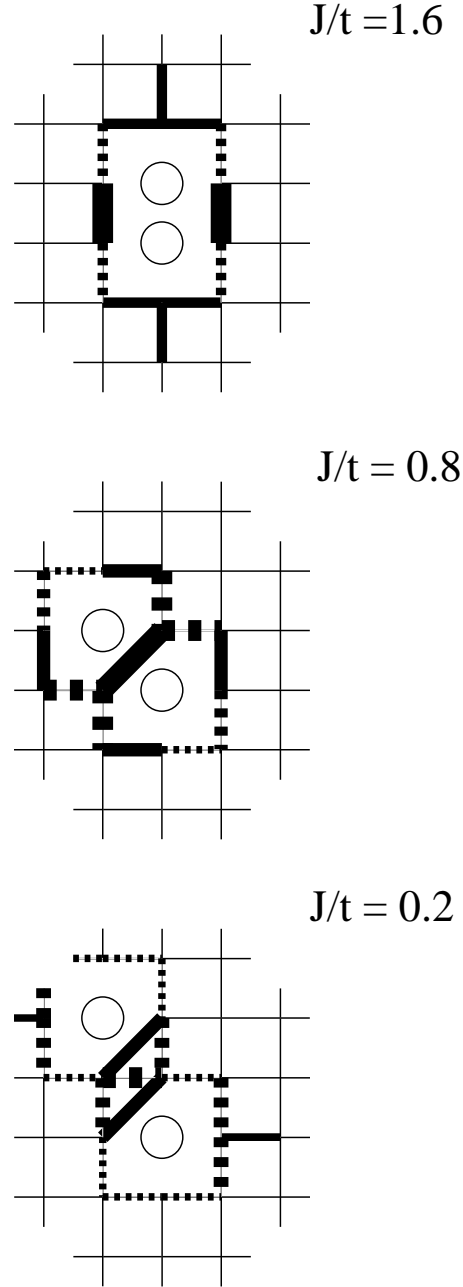


FIG. 10. Results for two holes obtained at several couplings  $J/t$  on a 20 sites square cluster using the Exact Diagonalization technique. The holes are fixed at the position with the highest chances in the ground state. Working in this subspace, bonds where the nearest-neighbor spin-spin correlation has the largest variation with respect to the undoped case are indicated. Solid (dashed) bonds indicate correlations which are larger (smaller) than in the undoped case by an amount larger than 20%. The thickness of the lines is proportional to the change observed. More than 20 sites in the clusters are shown for clarity (periodic boundary conditions were used).

and  $\sim -0.22$  at  $\lambda = 0.4$ . Then, the effect appears also in ladders and in this case it complements the tendency to form singlets which is natural in this type of geometry. In addition, similar studies for the case  $\lambda = 0$  have allowed us to verify that in the subspace of  $s$ -wave states the diagonal singlet is now a *triplet*, also in agreement with the predictions of Sec.II. Then, this establishes that the antiferromagnetic fluctuations and the  $d$ -wave character of the two-hole bound state contribute significantly to the formation of the diagonal strong spin singlet in ladders and planes.

#### IV. TRUNCATED LANCZOS

It would be interesting to check if the results obtained in the previous section survive an increase in the lattice size, specially for the case of the two-dimensional clusters. *A priori* the strong similarities between the DMRG and ED results on small clusters for the case of 2-leg ladders suggest that the two-hole bound state is not much affected by size effects, at least for the case of tight pairs. Nevertheless, even if only for completeness, the issue of size effects is here addressed using the so-called “Truncated” Lanczos (TL) approach [22]. This technique is currently under development and it has the advantage of sharing the same good features of the ED method, specially (i) the ability of producing dynamical information, (ii) the generation of results using states with momentum as a good quantum number (e.g. if periodic boundary conditions are used), and (iii) the ability to study Hamiltonians that include interactions at intermediate and large distances if needed. Thus, in addition to verifying the results previously discussed, this section has as an extra goal the test of the TL method in a physically relevant case. Although it is doubtful that the TL method will reach the same accuracy of the DMRG approach in the study of static properties of quasi-one-dimensional systems, it may provide an intermediate algorithm between ED and DMRG keeping some of the main features of both techniques. Actually, recent developments [28] in this context using an exact change of basis to work with better degrees of freedom for the truncation procedure have already produced promising results that may transform the TL method into a more widely used technique for the study of correlated electrons.

Since the details of the Truncated Lanczos approach were described before in the literature [22], here only a brief summary will be included. In the first step of this method one state of the full basis (belonging to the subspace of momentum and total spin  $z$ -projection that will be investigated) is selected to start the iterations. In the analysis below the zero momentum Néel state was used. Note that this starting point is somewhat inefficient for the case of ladder systems where the ground state has no long-range order and a spin-gap, and the recent developments [28] mentioned before have indicated that a better

starting point would be to use rung spin singlets in the singlet-triplet basis. Nevertheless, for the particular case of two holes in the  $t - J$  model the approach in the  $S^z$ -basis seems accurate (as shown below) and, thus, results in the new basis will be postponed for a future publication. After the initial state is chosen, the Hamiltonian is applied several times producing a basis set of a few hundred states. In this space, generated dynamically by the Hamiltonian, a Lanczos diagonalization is performed. The ground state wave function is analyzed and only the basis states with a weight  $|c|^2 > \lambda$  are kept. The cutoff  $\lambda$  is selected such that the number of states after the truncation procedure is performed is only about 50% or less of the size of the matrix being studied. The procedure is repeated several times i.e. growing the space, diagonalizing in the generated basis, truncating to a fraction of it (“back and forth” procedure), until the available amount of memory is exhausted. This slow-growth approach has proven to work very well in some cases such as the  $t - J_z$  model [22], and it is believed to produce reasonable results in spin-gapped models. However, below it will be shown that it works also for two-dimensional clusters that have low-energy excitations.

##### A. Truncated Lanczos on Ladders

Fig.11 shows the ground state energy as a function of the size of the basis for a  $2 \times 16$  cluster with 2 holes. This particular example can not be solved exactly with present day computers since the total Hilbert space contains  $\sim 10^9$  states, even after translational invariance is used to reduce the basis size. However, Fig.11 suggests that the

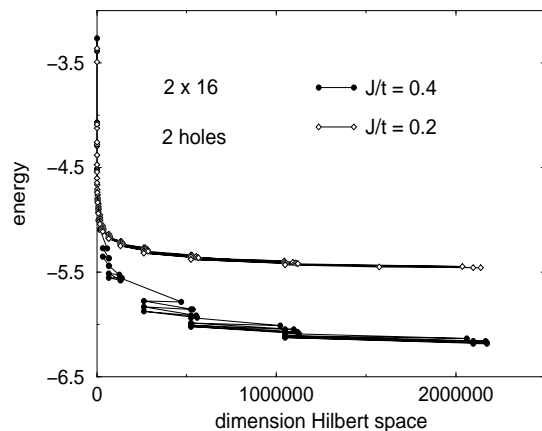


FIG. 11. Ground state energy obtained using the Truncated Lanczos approach working at  $J/t = 0.2$  and  $0.4$ , as a function of the size of the basis used. The cluster has  $2 \times 16$  sites and there are two holes. The oscillations are produced by the “back and forth” procedure described in the text. For both couplings the energy is measured with respect to the energy of the Néel state with two holes in the same rung, namely  $E = -J(48 - 5)/2$ .

TL approach with only  $\sim 2 \times 10^6$  states produces an energy converged up to 3 significant figures. The oscillations in the energy shown in Fig.11 as the dimension of the Hilbert space grows are a consequence of the “back and forth” procedure described before.

In the absence of an exact value for the ground state energy of the cluster considered in Fig.11, it is possible to judge the accuracy of the approximate state obtained using the TL method by evaluating correlation functions. In Fig.12 a calculation similar to that reported in Fig.7 is presented, namely fixing  $J/t$  the configuration of holes with the highest chances is selected, and in that subspace the spin correlations in the vicinity of the holes are shown. The links where the nearest-neighbor spin-spin correlation functions have the largest variation with respect to the undoped system (also calculated with the TL method) are highlighted. Qualitatively the results are very similar to those found using the  $2 \times 10$  cluster, i.e. for  $J/t = 0.4$  the  $\sqrt{2}$  hole configuration has the highest chances and the spin singlet along the opposite diagonal is strong, while for  $J/t = 0.2$  the holes are at distance  $\sqrt{5}$  with two spin singlets formed in between. The excellent agreement between the results obtained with the TL method compared with ED and DMRG techniques is somewhat surprising since in the TL method applied to the  $S^z$  basis the spin-spin correlations away from the holes indicate correlations stronger than expected for a spin-gapped system. However, in spite of this fact the behavior of holes is not affected, reinforcing the notion that the physics of tight hole pairs is dominated by the presence of spin correlations at short distances independently of their long-range behavior. Similar conclusions

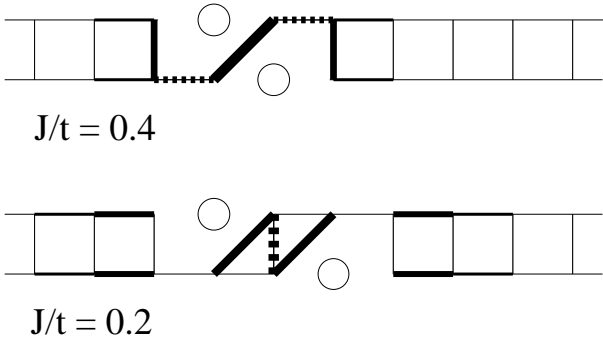


FIG. 12. Results for two holes obtained at several couplings  $J/t$  on a  $2 \times 16$  cluster using the Truncated Lanczos algorithm keeping  $\sim 2 \times 10^6$  states. The holes are fixed at the position with the highest chances in the ground state. Working in this subspace, bonds where the nearest-neighbor spin-spin correlation has the largest variation with respect to the undoped case are indicated. Solid (dashed) bonds indicate correlations which are larger (smaller) than in the undoped case by an amount larger than 20%. The thickness of the lines is proportional to the change observed.

can be reached analyzing other observables. For instance,

Fig.13 shows  $P(d)$  for the  $2 \times 16$  cluster, and a couple of couplings. Several distances have comparable probabilities. In particular for  $J/t = 0.2$  there is an approximate plateau in  $P(d)$  between  $d = 1$  and 3.

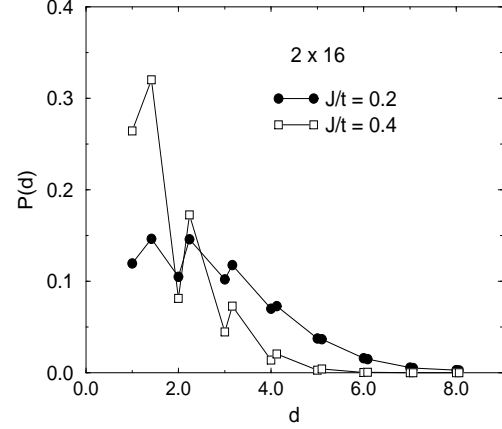


FIG. 13. Probability  $P(d)$  of finding the holes at a distance  $d$  on a  $2 \times 16$  cluster with two holes, calculated using the Truncated Lanczos algorithm. Results for two couplings  $J/t$  are presented.

## B. Truncated Lanczos on 2D Clusters

Encouraged by these results, the TL approach was applied to the 2D  $\sqrt{32} \times \sqrt{32}$  cluster with 2 holes. Although the basis needed to solve exactly this problem can be reduced by a factor 4 compared with the basis used for the ladder (due to rotational invariance on square clusters), the problem is difficult to solve exactly [29] and in addition it has not been addressed with DMRG techniques. Fig.14 contains TL results using  $\sim 2 \times 10^6$  states isolating the hole configuration with the highest chances and studying the spin background in its vicinity. Once again, the results are almost identical to those found using smaller clusters (Fig.10). The dynamically generated strong plaquette-diagonal spin singlet clearly appears in the 2D cluster study, similarly as it occurs in 2-leg ladders. Fig.15 shows that the same agreement with smaller cluster calculations occurs once the hole-hole correlation  $\langle n(0)n(\mathbf{r}) \rangle$ , where  $n(\mathbf{r})$  is the hole number operator at site  $\mathbf{r}$ , is calculated. For  $J/t = 0.4$  the correlation is maximized at distance  $\sqrt{2}$ . However, remember that a given site has 4 neighbors at distance  $\sqrt{2}$  but 8 at distance  $\sqrt{5}$ , and thus the maximum probability  $P(d)$  is at  $d = \sqrt{5}$  in the case of  $J/t = 0.2$ . Fig.16 shows similar information in a different representation. The results are in good qualitative agreement with those found in smaller clusters.

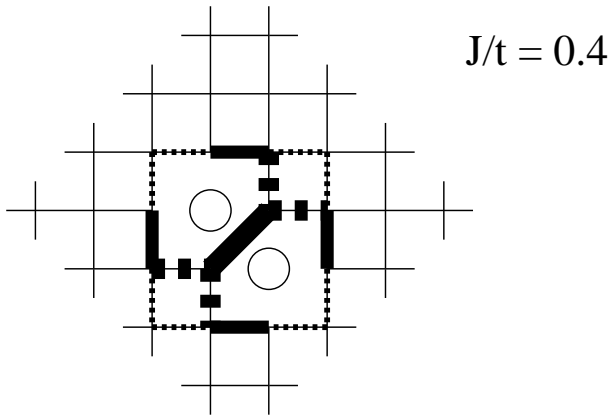


FIG. 14. Results for two holes obtained at  $J/t = 0.4$  on a 32 sites square cluster using the Truncated Lanczos algorithm keeping  $\sim 2 \times 10^6$  states. The holes are fixed at the position with the highest chances in the ground state. Working in this subspace, bonds where the nearest-neighbor spin-spin correlation has the largest variation with respect to the undoped case are indicated. Solid (dashed) bonds indicate correlations which are larger (smaller) than in the undoped case by an amount larger than 20%. The thickness of the lines is proportional to the change observed.

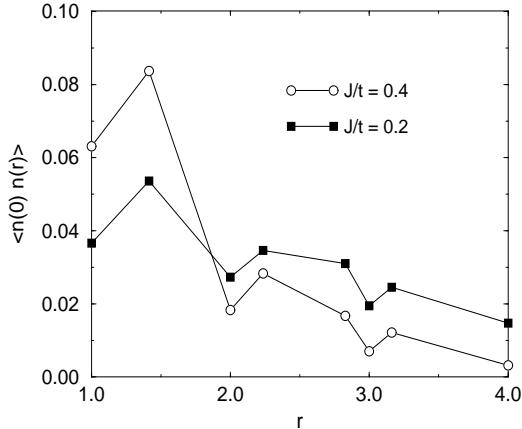


FIG. 15. Hole-hole correlation  $\langle n(0)n(r) \rangle$  vs distance  $r$  obtained with the Truncated Lanczos method on a 32 sites square cluster and two holes keeping  $\sim 2 \times 10^6$  states. The couplings are indicated.

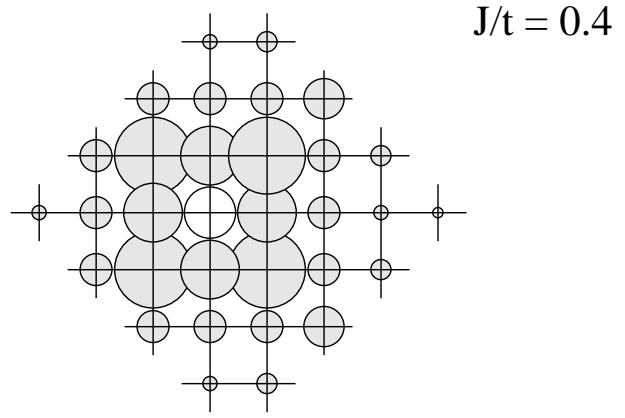


FIG. 16. Ground state results obtained on a 32 sites square cluster with two holes at  $J/t = 0.4$  using the Truncated Lanczos algorithm keeping  $\sim 2 \times 10^6$  states. One hole is fixed at the position denoted by the open circle. The area of the gray circles is proportional to the probability of finding the other hole at a particular site.

## V. INFLUENCE OF HOLE-HOLE ELECTROSTATIC REPULSION

Results such as those contained in Figs.6,9 and 16 clearly imply that a pair of holes form a bound state on 2-leg ladders and planes in the realistic regime of couplings close to  $J/t \sim 0.4$ , in agreement with a vast amount of previous literature [4]. At this coupling the “size” of the pair (defined as the mean distance between holes) is about a couple of lattice spacings. Since for  $J/t = 0.2$ , the bound state seems to have disappeared (according again to the same Figures), then the pair size must change very rapidly in the window of couplings between 0.2 and 0.4, where a “critical” value  $J/t|_c$  must exist leading to hole binding.

Let us analyze in more detail a particular case such as  $J/t = 0.4$  which is located in a window of couplings “a priori” presumed to be realistic. Here holes are mainly located at distances 1,  $\sqrt{2}$ , and  $\sqrt{5}$  lattice spacings from each other. Such small distances naturally raise a couple of concerns: first, experimental results for YBCO have suggested that its coherence length  $\xi$  is about  $15\text{\AA}$  which roughly corresponds to 4 lattice spacings [5]. Doped La-cuprates have an even higher  $\xi$  of about  $35\text{\AA}$ . More recent estimations arrive to  $\xi = 18.3\text{\AA}$  and  $22.7\text{\AA}$  for 1% Zn-doped underdoped YBCO and La-214, respectively [30]. These lengths are certainly much shorter than those observed in low temperature superconductors, but still do not locate the cuprates in the regime where  $\xi$  is smaller than the mean distance between carriers. If  $\xi$  is interpreted, as usually done, as the size of the Cooper pairs in the superconducting condensate and if the  $t - J$  model is used, then  $J/t$  must be fine-tuned closer to its critical value  $J/t|_c$  to have hole pairs of size equal to the experimentally measured  $\xi$ . In other words, at  $J/t = 0.4$  the hole pairs in the  $t - J$  model are substantially smaller in

size than needed to represent the cuprates. Then, from this point of view the peculiar properties of a very tight bound state are not much relevant, and only the qualitative aspects of the problem can be extracted from studies of the pure  $t - J$  model at  $J/t = 0.4$ .

In addition, having pairs of small size raises concerns regarding the stability of such pairs once the Coulomb interaction is considered. While the on-site electronic repulsion is usually taken into account in the framework of strongly correlated electrons, the repulsion at the next relevant distance of one lattice spacing is usually neglected (with an exception being the analysis of stripe formation in the cuprates [31]). Other authors have raised similar concerns [32]. A rapid estimation shows that the Coulombic electrostatic effect cannot be neglected since the bare potential energy between two charges at one lattice spacing from each other is  $V_{NN} = e^2/a = 3.8 \text{ eV}$ , where  $a = 3.8 \text{ \AA}$  as in the Cu-oxides compounds. Certainly this repulsion is considerably larger than the attraction expected between holes which is regulated by  $J \sim 0.1 \text{ eV}$ . This source of attraction would be destroyed by the bare Coulomb interaction, unless retardation effects are important.

However, it is reasonable to consider a more optimistic scenario where the Coulomb repulsion at distance of one lattice is influenced by other orbitals in the Cu-ions, polarization of oxygen [33], and possible metallic screening in the doped regime. To gain some intuitive insight about the influence of these effects let us first simply divide  $V_{NN}$  by the dielectric constant  $\epsilon_\infty$  obtained experimentally for the high-Tc compounds (certainly being aware that the result will be qualitative at best since one is not supposed to use such a constant for the short distance effects discussed in this section). Although there is a large range of estimations in the literature, a number near  $\epsilon_\infty \sim 30 - 40$  is a reasonable assumption [34]. However, even considering this factor the new estimation of the Coulomb repulsion still gives a number competing with the order of magnitude of the attraction caused by antiferromagnetism, namely  $V_{NN} = e^2/(\epsilon_\infty a) = 0.1 \text{ eV}$ . A variety of other calculations lead to qualitatively similar results. The Cu-O repulsion ( $V_{pd}$ ) has been estimated to be  $\sim 1.0 \text{ eV}$  [35], i.e. smaller than the bare Coulomb interaction at distance  $1.9 \text{ \AA}$  roughly by a factor 8. If this same factor is applied at distance of one lattice spacing the Cu-Cu repulsion ( $V_{dd}$ ) should be about  $0.5 \text{ eV}$ . In addition, note that the binding energy of a hole pair in two-dimensional clusters for  $J/t = 0.4$  is only  $\Delta_B \sim 0.2J$  [4] i.e. while the hole attraction is regulated by  $J$  the numerical coefficient that takes into account the fact that holes actually lose kinetic energy by forming the pair magnifies even more the damaging effects of the Coulombic repulsion.

Then, electrostatic effects will likely make unstable the very tight pairs observed in the computer simulations described before. To analyze explicitly this effect in Fig.17 results for the probability of finding the holes at a given distance  $d$  are provided for the case of a 2-leg ladder [36].

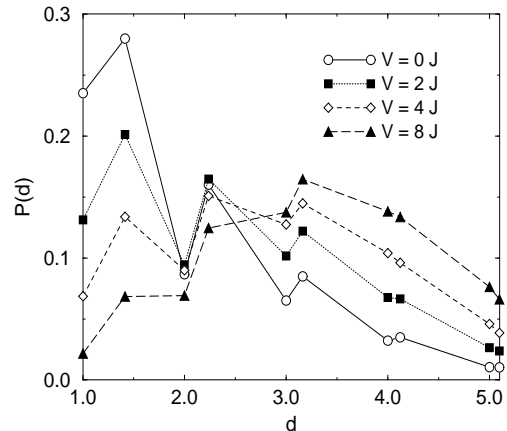


FIG. 17. Probability  $P(d)$  of finding the holes at a distance  $d$  on a  $2 \times 10$  cluster with two holes at  $J/t = 0.4$ , calculated using the Lanczos algorithm. Results for several values of the coupling  $V$  regulating a nearest-neighbor repulsion between holes are presented.

The Coulomb repulsion is included adding to the  $t - J$  Hamiltonian a term  $V \sum_{\langle ij \rangle} n_i n_j$ , where  $n_i$  is the number operator at site  $i$  and the rest of the notation is standard. The results show that the relevance of very small distances is actually lost already when  $V = 2J \sim 0.2 \text{ eV}$ . At larger values of the repulsion such as  $V = 4J$  the probability has a broad plateau between distances 2 and 3, and the bound state seem to disappear when  $V$  is increased slightly further [37]. Note, however, that if the hole-hole instantaneous Coulombic repulsion is assumed to be short-ranged more extended bound states may survive the inclusion of such electrostatic energies since their size increases as  $J/t$  is reduced to its critical value. But this once again will imply that a typical bound state size will be larger than just a couple of lattice spacings.

There are two possible ways to avoid the problem of the Coulomb interaction at short distances. One is by considering retardation effects, and the other by finding other sources of screening that could reduce drastically the previous estimations of  $V_{NN}$ . Let us consider retardation first: the discussion in the previous sections have indeed suggested that this effect is important in the  $t - J$  model and it may avoid the problem of the Coulombic interaction similarly as it occurs in electron-phonon systems, namely a hole could scramble the spin order in a region of space during its movement, and a second hole could take advantage of this distortion. If one hole follows the other at a distance of a few lattice spacings, then the short-distance Coulomb repulsion can be avoided and the results would be compatible with estimations of  $\xi$  in the literature. As a simple illustration in Fig.18, a hole creates a string excitation [38] and a second hole heals the damage in the spin background at a later time [39],

but keeping some distance to avoid repulsions. A similar process can potentially take place in the case of ladders as also shown schematically in Fig.18. Considering the ground state as dominated by rung singlets, the movement of a hole produces the transformation of one of those singlets into a singlet along the diagonal of a plaquette. Then, moving a hole introduces a damage in the spin configuration similar to what occurs with strings in the planes. The second hole can heal this damage as shown in Fig.18.

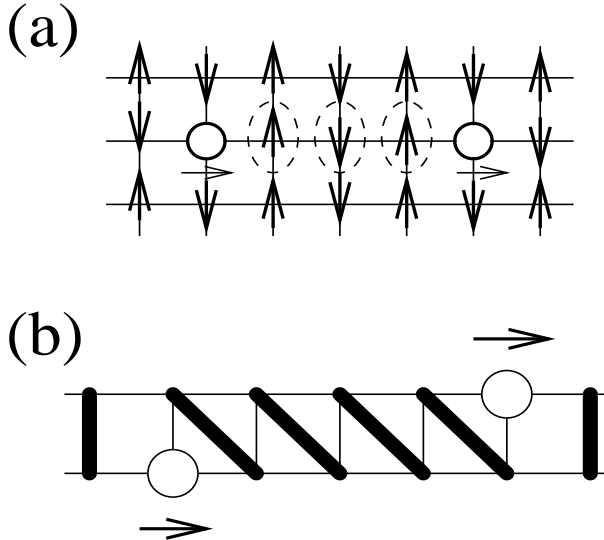


FIG. 18. (a) Possible behavior of holes in an antiferromagnetic background that avoids the short distance Coulombic repulsion. The first hole moving, e.g., to the left creates a string of spins (highlighted in the figure) incorrectly aligned with respect to the background. The second hole can heal this damage following the first hole at some distance. The picture is possible if the spin excitations have a large lifetime such that the string of spins is not erased by spin fluctuations before it is used by the second hole to improve its energy; (b) Similar ideas as in (a) but now in the context of ladders. Here the spin background is not antiferromagnetic but the spins mainly form singlets along the rungs. A hole moving along the chains creates a string of diagonal singlets. The second hole can heal this damage, keeping some distance from the first to avoid the Coulombic repulsion.

The second possible solution invokes a source of screening not considered in the previous discussion. In the absence of other holes and using the  $t - J$  model where electron-hole pairs cannot be created, metallic screening effects should not affect the results and, thus, the Coulombic interaction will actually be of long-range. However, in the presence of a finite density of holes, a simple Thomas-Fermi approximation can be used to make a rough estimation of a possible metallic screening length  $\lambda$ . Considering a hole density  $n \sim 7 \times 10^{21} \text{cm}^{-3}$  [5], and using standard textbooks equations for three dimensional metals,  $\lambda$  is found to be  $\sim 0.8 \text{\AA}$ , which is small indeed and could potentially drastically

reduce the effects of the Cu-Cu Coulomb interaction. However, it is clear that the Cu-oxides are very different from the three dimensional metals where Thomas-Fermi approximations are qualitatively reliable. Thus, the issue of whether metallic screening can reduce the effects of Coulomb repulsions between holes in the cuprates remains an open question that deserves further studies.

## VI. CONCLUSIONS

In this paper the problem of two holes in a spin background with robust antiferromagnetic correlations was revisited. Using Exact Diagonalization and Truncated Lanczos techniques applied to planes and ladders with up to 32 sites the typical distances between holes was studied. It was observed that the maximum probability occurs when the holes are at  $\sqrt{2}$  lattice spacings of each other, in agreement with previous calculations. However, other distances were found to be equally relevant. An intuitive explanation for these results in a real-space picture, as well as diagrammatically was provided. Strong spin singlets are found near two holes in a  $d$ -wave state. An explanation for this effect based on a Néel background was presented, complementing other approaches [19] based on spin disordered backgrounds. It is concluded that holes in their movement create spin excitations with a non-negligible lifetime, and thus *retardation* effects are important in the  $t - J$  model. However, the instantaneous approximation captures properly the qualitative aspects, specially the symmetry of the bound states which is in the  $d_{x^2-y^2}$  channel. The short size of the pairs raises concerns regarding the stability of the bound states if  $NN$  Coulomb interactions are included. Estimations of the strength  $V_{NN}$  of these interactions were here provided. A numerical study showed that the bound states increase their size as  $V_{NN}$  grows, and the typical hole distance in the pair can become comparable to the experimentally measured coherence length, which is about 4 lattice spacings, even if the values of  $J/t$  used produced unrealistic small pairs in the absence of the  $NN$  repulsion.

## VII. ACKNOWLEDGMENTS

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- [1] D. J. Scalapino, E. Loh, and J. E. Hirsch, Phys. Rev. **B** **34**, 8190 (1986). See also K. Miyake, S. Schmitt-Rink, and C. M. Varma, Phys. Rev. **B** **34**, 6554 (1986).

- [2] D. Pines, preprint, cond-mat 9704102, and references therein.
- [3] A. Kampf, and J. R. Schrieffer, Phys. Rev. **B 42**, 7967 (1990); and references therein.
- [4] For a review see E. Dagotto, Rev. Mod. Phys. **66**, 763 (1994).
- [5] M. Cyrot and D. Pavuna, *Introduction to Superconductivity and High-Tc Materials*, World Scientific (1992).
- [6] D. J. Scalapino, Phys. Rep. **250**, 331 (1995).
- [7] D. Poilblanc, J. Riera, and E. Dagotto, Phys. Rev. **B 49**, 12318 (1994); D. Poilblanc, Phys. Rev. **B 48**, 3368 (1993); and references therein. See also R. Eder, Phys. Rev. **B 45**, 319 (1992); P. Wróbel and R. Eder, Phys. Rev. **B 49**, 1233 (1994); and references therein.
- [8] A. Nazarenko, A. Moreo, J. Riera and E. Dagotto, Phys. Rev. **B 54**, R768 (1996).
- [9] D. S. Marshall, et al., Phys. Rev. Lett. **76**, 4841 (1996); H. Ding et al., Nature **382**, 51 (1996); H. Ding et al., Phys. Rev. Lett. **78**, 2628 (1997); S. LaRosa, I. Vobornik, H. Berger, G. Margaritondo, C. Kendziora, R.J. Kelley and M. Onellion, preprint.
- [10] S. Doniach et al., Phys. Rev. **B 41**, 6668 (1990); V. J. Emery et al., Nature **374**, 434 (1995); and references therein.
- [11] E. Dagotto, A. Nazarenko and A. Moreo, Phys. Rev. Lett. **74**, 310 (1995).
- [12] V. I. Belinicher, A. L. Chernyshev, and V. A. Shubin, Phys. Rev. **B 56**, 3381 (1997). See also A. V. Dotsenko, cond-mat/9612215
- [13] For a recent review see E. Dagotto and T. M. Rice, Science **271**, 618 (1996).
- [14] S. R. White, R. M. Noack, and D. J. Scalapino, Phys. Rev. Lett. **73**, 886 (1994).
- [15] M. Sigrist, T. M. Rice, and F. C. Zhang, Phys. Rev. **B 49**, 12058 (1994).
- [16] H. Tsunetsugu, M. Troyer, and T. M. Rice, Phys. Rev. **B 49**, 16078 (1994).
- [17] E. Dagotto, J. Riera, and D. J. Scalapino, Phys. Rev. **B 45**, 5744 (1992).
- [18] S. R. White, Phys. Rev. Lett. **69**, 2863 (1992).
- [19] S. R. White and D. J. Scalapino, Phys. Rev. **B 55**, 6504 (1997).
- [20] P. W. Anderson, Mater. Res. Bull. **8**, 153 (1973). See also S.A. Kivelson, D.S. Rokhsar, and J.P. Sethna, Phys. Rev. **B 35**, 8865 (1987).
- [21] D. Poilblanc, Phys. Rev. **B 49**, 1477 (1994).
- [22] J. Riera and E. Dagotto, Phys. Rev. **B 47**, 15346 (1993); J. Riera and E. Dagotto, *ibid* **B 48**, 9515 (1993); and references therein.
- [23] G. Sierra et al., preprint, cond-mat/9707335. See also G. Sierra and M. A. Martin-Delgado, preprints, cond-mat/9704212 and cond-mat/9706104.
- [24] For recent results in this context see R. Fye, preprint, cond-mat/9706073 and references therein.
- [25] S.-C. Zhang, Science **275**, 1089 (1997).
- [26] Other problems with the SO(5) scenarios have been discussed by M. Greiter, preprint, cond-mat/9705049, and G. Baskaran and P. W. Anderson, preprint, cond-mat/9706076.
- [27] On the cluster of 16 sites the ground state of two holes is *d*-wave for all the values of  $\lambda$  investigated here. For the case of 20 sites, note that the *s* and *d* character of the undoped and two hole ground states are interchanged with respect to the 16 site cluster. This effect appears even in  $2 \times 2$  clusters and it is not a problem since the operator that links the undoped and two-hole cases is always *d*-wave. For details see A. Moreo and E. Dagotto, Phys. Rev. **B 42**, 2347 (1990). See also S. Trugman and D. J. Scalapino, preprint, and Ref. [19].
- [28] E. Dagotto, G. Martins, J. Piekarewicz, J. Riera, and J. R. Shepard, preprint, cond-mat/9707205.
- [29] Nevertheless this case is solvable exactly with the Lanczos method (P. Leung, private communication).
- [30] B. Nachumi et al., Phys. Rev. Lett. **77**, 5421 (1996).
- [31] V. J. Emery, and S. A. Kivelson, Physica **C 209**, 597 (1993); U. Löw et al., Phys. Rev. Lett. **72**, 1918 (1994); S. Haas et al., Phys. Rev. **B 51**, 5989 (1995); and references therein.
- [32] D. Mihailovic and K. A. Müller, Proc. NATO ASI, *Materials aspects of High-Tc Superconductivity 10 years after the discovery*, to be published by Kluwer, 1997. See also G. Baskaran and P. W. Anderson, cond-mat/9706076 in their criticism of the SO(5) unification attempt.
- [33] S. Ishihara, M. Tachiki, and T. Egami, Phys. Rev. **B 49**, 16123 (1994), and references therein. See also D. K. G. de Boer, C. Haas, and G. A. Sawatzky, Phys. Rev. **B 29**, 4401 (1984); J. van den Brink, M. B. J. Meinders, J. Lorenzana, R. Eder and G. A. Sawatzky, Phys. Rev. Lett. **75**, 4658 (1995).
- [34] C. Y. Chen et al., Phys. Rev. Lett. **63**, 2307 (1989); D. Reagor et al., Phys. Rev. Lett. **62**, 2048 (1989).
- [35] M. S. Hybertsen et al., Phys. Rev. **B 41**, 11068 (1990); M. Schlüter and M. S. Hybertsen, Physica **C162-164**, 583 (1989); A. K. McMahan, J. F. Annett, and R. M. Martin, Phys. Rev. **B 42**, 6268 (1990); and references therein. See also L. H. Tjeng, H. Eskes, and G. A. Sawatzky, in *Strong Correlation in Superconductivity*, Eds. H. Fukuyama, S. Maekawa, and A. P. Malozemoff, Springer series in Solid-State Sciences, Vol. 89 (1989) and H.-B. Schüttler and A. J. Fedro, Phys. Rev. **B 45**, 7588 (1992).
- [36] Previous results for the case of two-dimensional *t*-*J* clusters with Coulomb repulsion can be found in T. Barnes and M. D. Kovarik, Phys. Rev. **B 42**, 6159 (1990). Results for the multiband Hubbard model with Coulomb repulsions are in J. Riera and E. Dagotto, Phys. Rev. **B 50**, 3215 (1994).
- [37] Note that similar calculations carried out in two dimensional clusters that can be solved exactly are more severely affected by size effects. Nevertheless the tendency to maximize the distance between holes upon the introduction of the nearest-neighbor Coulomb repulsion is clear.
- [38] B. Shraiman and E. Siggia, Phys. Rev. Lett. **60**, 740 (1988). See also E. Dagotto et al., Phys. Rev. **B 41**, 9049 (1990), and references therein.
- [39] This picture was discussed before in J. Hirsch, Phys. Rev. Lett. **59**, 228 (1987).